Stochastic Approach To Non-Equilibrium Quantum Spin Systems

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Outline

- Introduction to stochastic approach
- Utility in and out of equilibrium
- Thermodynamics of a single cluster of spins
- Dynamics of quantum Heisenberg models
- Dynamical quantum phase transitions
- Stochastic approach for quantum Ising model
- Signatures of DQPTs in classical approach
- Other observables, non-integrable, higher dimensions
- Current status and future developments

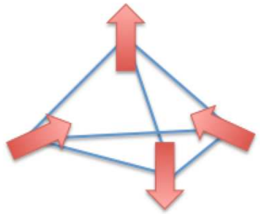
Single Cluster of Quantum Spins

Hogan and Chalker, *Path integrals, diffusion on SU(2) and the fully frustrated antiferromagnetic spin cluster*, J. Phys. A **37**, 11751 (2004)

$$\hat{H} = \frac{J}{2}\left(\sum_{i=1}^{q} \hat{\mathbf{S}}_i\right)^2 \equiv \frac{J}{2}\hat{\mathbf{S}}_{\mathrm{T}}^2$$

Partition function of a single cluster of q spins

$$Z = \mathrm{Tr}\left(e^{-\beta \hat{H}}\right)$$



Hubbard–Stratonovich transformation

$$e^{-\frac{1}{2}\beta J \hat{\mathbf{S}}_{\mathrm{T}}^2} = \int \mathcal{D}\mathbf{h}(\tau) \exp\left\{-\int_0^\beta d\tau \left(\frac{1}{2J}\mathbf{h}^2(\tau) + i\mathbf{h}(\tau).\hat{\mathbf{S}}_{\mathrm{T}}\right)\right\}$$

Single spin S in a stochastic magnetic field

Evolution operator for a single spin in a time-dependent field

$$\hat{\mathrm{T}}(t) = \mathbb{T}\exp\left\{-i\int_0^t d\tau\, \mathbf{h}(\tau).\hat{\mathbf{S}}\right\}$$

Diffusion on SU(2)

$$Z = \int \mathcal{D}\mathbf{h}(\tau) \exp\left\{-\int_0^\beta d\tau \, \frac{1}{2J}\mathbf{h}^2(\tau)\right\} [\mathrm{Tr}\, \hat{\mathrm{T}}(\beta)]^q$$

$$\langle \ldots \rangle|_{t=\beta} \equiv \int \mathcal{D}\mathbf{h}(\tau) \ldots e^{-\int_0^\beta d\tau \, \frac{1}{2J}\mathbf{h}^2(\tau)}$$

$$Z = \left\langle \left[\mathrm{Tr}\, \hat{\mathrm{T}}(t)\right]^q \right\rangle\Big|_{t=\beta}$$

Euler angle parametrization

$$\hat{\mathrm{T}}(\alpha, \beta, \gamma; t) = e^{-i\alpha(t)\hat{S}_3} e^{-i\beta(t)\hat{S}_2} e^{-i\gamma(t)\hat{S}_3}$$

Langevin equations for stochastic evolution of coordinates

$$\dot{\alpha} = h_1(t)(-\cos\alpha \cot\beta) + h_2(t)(-\sin\alpha \cot\beta) + h_3(t)$$

$$\dot{\beta} = h_1(t)(-\sin\alpha) + h_2(t)(\cos\alpha)$$

$$\dot{\gamma} = h_1(t)(\cos\alpha \,\mathrm{cosec}\,\beta) + h_2(t)(\sin\alpha \,\mathrm{cosec}\,\beta)$$

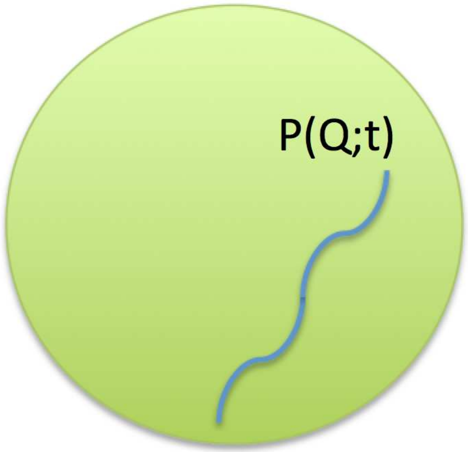
$$m\frac{d\mathbf{v}}{dt} = -\gamma\mathbf{v} + \boldsymbol{\eta}(t)$$

Langevin to Fokker–Planck

Stochastic Langevin to deterministic Fokker-Planck

Probability distribution for the end points of the evolution

$$Q \equiv (\alpha, \beta, \gamma)$$



$$Z = \int d\tau_Q \, \mathrm{P}(Q;t)[\mathrm{Tr}\,\hat{\mathrm{T}}(Q;t)]^q|_{t=\beta}$$

Fokker-Planck Equation

Probability $\mathrm{P}(\alpha, \beta, \gamma; t)$ of coordinates α, β, γ

$$\partial_t \mathrm{P}(\alpha, \beta, \gamma; t) = \tfrac{J}{2} \nabla^2 \mathrm{P}(\alpha, \beta, \gamma; t)$$

Laplace-Beltrami operator on $SU(2)$

$$\nabla^2 = \mathrm{cosec}\beta \partial_\beta \sin\beta \partial_\beta + \mathrm{cosec}^2\beta [\partial_\alpha^2 + \partial_\gamma^2 - 2\cos\beta \partial_\alpha \partial_\gamma]$$

Eigenfunctions and eigenvalues are known

$$Z = \sum_j e^{-\frac{1}{2} j(j+1)\beta J} (2j+1) \times$$

$$\frac{2}{\pi} \int_0^\pi d\psi \left\{ \frac{\sin[(2S+1)\psi]}{\sin\psi} \right\}^q \sin[(2j+1)\psi] \sin\psi$$

Exact partition function via Hubbard-Stratonovich

$$\boxed{Z = \sum_j e^{-\beta E_j} g_j}$$

E_j energy levels $\quad$ g_j degeneracies $\quad$ $2j \in \mathbb{Z}_0^+$

Dynamics of Spin Models

Ringel and Gritsev, *Dynamical symmetry approach to path integrals of quantum spin systems*, Phys. Rev. A **88**, 062105 (2013)

Galitski, *Quantum-to-Classical Correspondence and Hubbard-Stratonovich Dynamical Systems, a Lie-Algebraic Approach*, Phys. Rev. A **84**, 012118 (2011)

$$\hat{H} = \sum_{ij} J_{ij}^{ab} \hat{S}_i^a \hat{S}_j^b + \sum_i h_i^a \hat{S}_i^a$$

Condensed matter, cold atoms, quantum information ...

Spins $\hat{S}_j^a$ on site j obey $\boxed{[\hat{S}_j^a, \hat{S}_{j'}^b] = i\delta_{jj'}\epsilon^{abc}\hat{S}_j^c}$ with $\hbar = 1$

Here J_{ij}^{ab} is the exchange interaction and h_i^a is an applied field

Dynamics of model governed by time evolution operator

$$\hat{U}(t_f, t_i) = \mathbb{T} \exp\left(-i \int_{t_i}^{t_f} \mathrm{d}t\, \hat{H}(t)\right)$$

Initial and final times t_i and t_f $\quad \hat{H}(t)$ can be time-dependent

Time Evolution Operator

$\hat{U}(t_f, t_i)$ non-trivial due to interactions between the spins, non-commutativity of spin operators and time ordering $\mathbb{T}$

$$\hat{U}(t_f, t_i) = \mathbb{T} \exp\left(-i \int_{t_i}^{t_f} \mathrm{d}t\, \hat{H}(t)\right)$$

However, $\hat{U}$ can be transformed via exact transformations

Interactions decoupled using Hubbard–Stratonovich transformations over auxiliary variables ϕ_i^a:

$$\hat{U} = \mathbb{T} \int \mathcal{D}\phi \, \exp\left(-iS - i \int_{t_i}^{t_f} \mathrm{d}t \sum_j (\phi_j^a \hat{S}_j^a + h_j^a \hat{S}_j^a)\right)$$

$\mathcal{D}\phi \equiv \prod_j \mathcal{D}\phi_j^a$ and normalization factors absorbed into measure

Decoupled spins interacting with stochastic fields ϕ_i^a

$$S = \frac{1}{4} \int_{t_i}^{t_f} \mathrm{d}t \sum_{ij} (J^{-1})_{ij}^{ab} \phi_i^a \phi_j^b$$

Disentangling

$$\hat{U}(t_f, t_i) = \left\langle \mathbb{T}\, e^{-i\int_{t_i}^{t_f} dt \sum_j \Phi_j^a(t)\hat{S}_j^a(t)} \right\rangle_\phi$$

$$\Phi_j^a \equiv \phi_j^a + h_j^a$$

Average $\langle \ldots \rangle_\phi$ taken with Gaussian "noise action"

Time-ordered exponential can be recast as a group element

$$\hat{U}(t_f, t_i) = \left\langle \prod_j e^{\xi_j^+(t_f)\hat{S}_j^+} e^{\xi_j^z(t_f)\hat{S}_j^z} e^{\xi_j^-(t_f)\hat{S}_j^-} \right\rangle_\phi$$

$$\hat{S}_j^\pm = \hat{S}_j^x \pm i\hat{S}_j^y$$

The coefficients ξ_j^a are *disentangling variables*

Related to the original Φ_j^a

Stochastic Differential Equations

Ringel and Gritsev, Phys. Rev. A **88**, 062105 (2013)

Disentangling variables satisfy SDEs

$$i\dot{\xi}_j^+ = \Phi_j^+ + \Phi_j^z \xi_j^+ - \Phi_i^- {\xi_j^+}^2$$

$$i\dot{\xi}_j^z = \Phi_j^z - 2\Phi_j^- \xi_j^+$$

$$i\dot{\xi}_j^- = \Phi_j^- \exp \xi_j^z$$

where $\Phi_j^a = \phi_j^a + h_j^a$ and initial conditions $\xi_i^a(t_i) = 0$

Non-linear SDEs for complex variables ξ_j^a, where Hubbard–Stratonovich variables ϕ_j^a are Gaussian noise

$$\frac{d\xi_i^a}{dt} = A_i^a(\{\xi_i\}) + \sum_{jb} B_{ij}^{ab}(\{\xi_i\})\bar{\phi}_j^b$$

A_i^a and B_{ij}^{ab} are drift and diffusion coefficients

$\{\xi_i\} = (\xi_i^z, \xi_i^{\pm})$, and $\bar{\phi}_j^b$ are delta-correlated white noise variables obtained by diagonalizing the noise action

Loschmidt

A natural quantity to study in the stochastic approach is the Loschmidt amplitude or return probability

Amplitude to return to initial state $|\psi(0)\rangle$ after time t

$$A(t) = \langle\psi(0)|\hat{U}(t)|\psi(0)\rangle$$

Evolution operator is centre stage

Loschmidt rate function

$$|A(t)|^2 = e^{-N\lambda(t)} \qquad \lambda(t) = -N^{-1}\ln|A(t)|^2$$

Dynamical Quantum Phase Transitions (DQPTs)

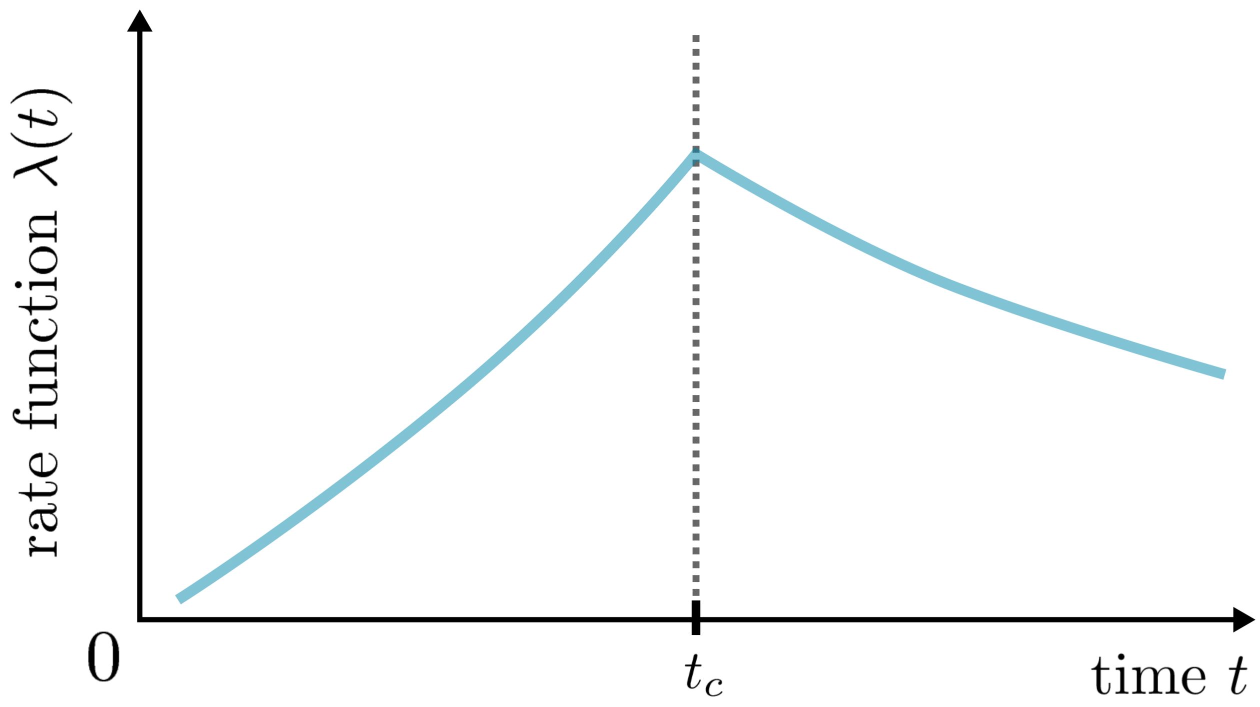
Compare with thermodynamic phase transitions

$$Z(T) = \mathrm{Tr}(e^{-\hat{H}/k_B T}) \qquad f = -k_{\mathrm{B}} T N^{-1} \ln Z(T)$$

Dynamical Quantum Phase Transitions

Heyl, Polkovnikov and Kehrein, *Dynamical Quantum Phase Transitions in the Transverse-Field Ising Model*, Phys. Rev. Lett. **110** 135704 (2013)

Non-analytic behavior at a critical time



Markus Heyl, *"Dynamical quantum phase transitions: a review"*, Rep. Prog. Phys. **81**, 054001 (2018)

Transverse Field Ising Model

In order to provide explicit results we consider TFI model

$$\hat{H}_{\mathrm{I}} = -J\sum_{j=1}^{N}\hat{S}_j^z\hat{S}_{j+1}^z - \Gamma\sum_{j=1}^{N}\hat{S}_j^x$$

N lattice sites, FM interactions $J > 0$, periodic boundaries

We set $J = 1$ and measure time in units of J

Initial FM state $\quad |\psi(0)\rangle = \otimes_j|\downarrow\rangle_j \equiv |\Downarrow\rangle$

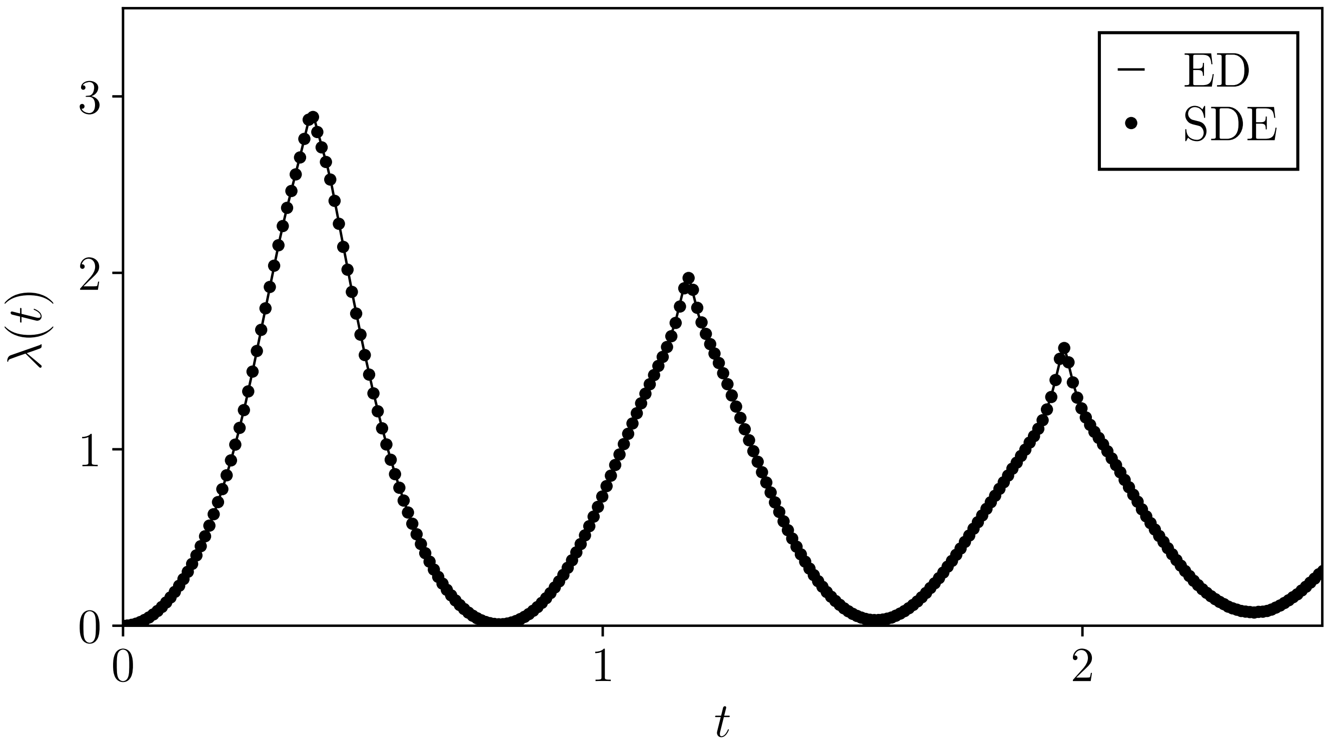
$$A(t) = \left\langle \prod_{j=1}^{N}\exp\left(-\frac{\xi_j^z(t)}{2}\right)\right\rangle_\phi$$

Disentangling variables $\xi_j^z(t)$ satisfy SDEs with the appropriate model specific Ising coefficients

Result for $A(t)$ holds for generic Heisenberg starting in $|\Downarrow\rangle$

Averaging over Trajectories

Clearly resolved Loschmidt peaks

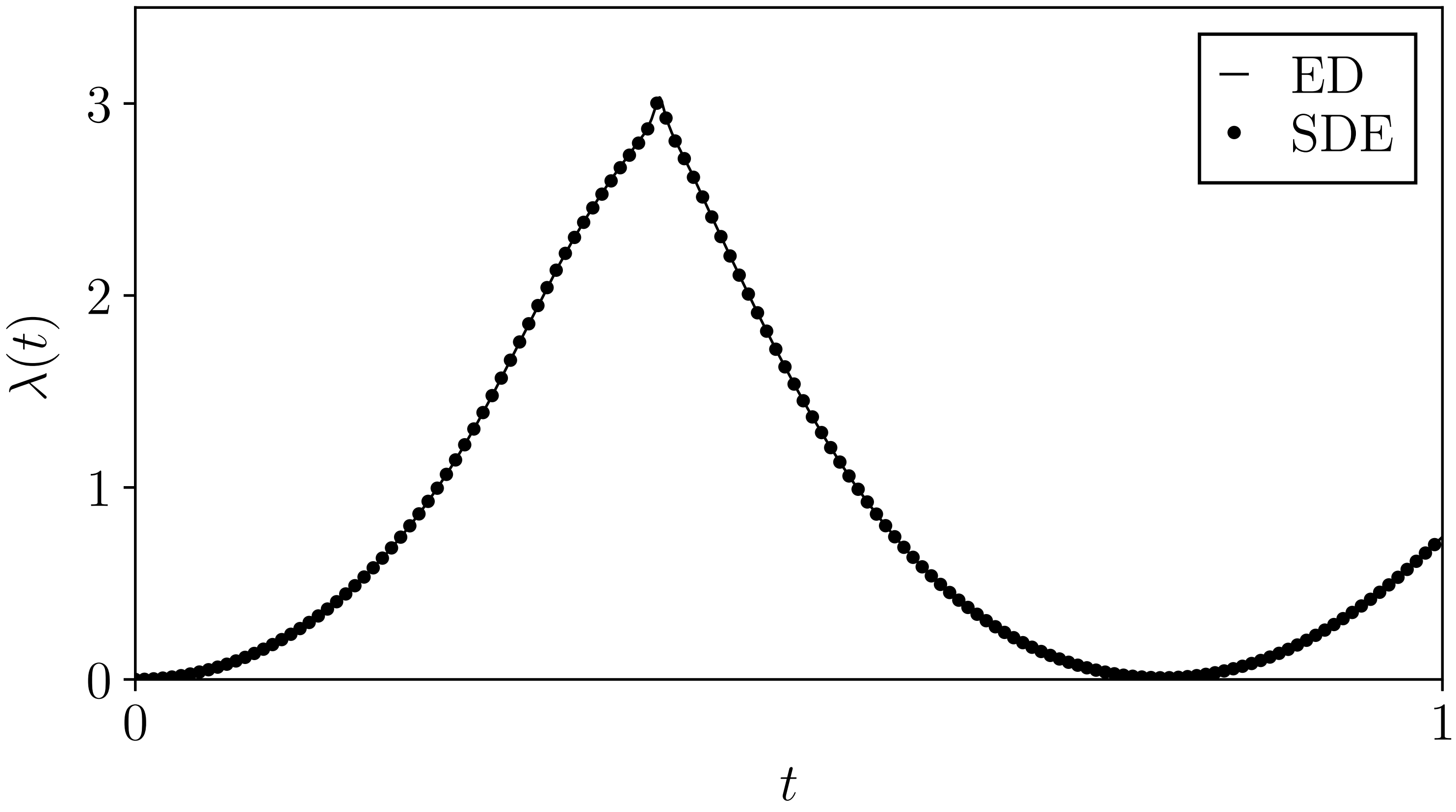


5×10^5 stochastic realizations with $dt = 10^{-5}$

Excellent agreement with ED for $N = 7$ spins

Larger System Sizes

$N = 14$ spins



3.2×10^6 stochastic realizations with $dt = 10^{-5}$

Role of Classical Variables

$$A(t) = \left\langle \prod_j \exp\left(-\frac{\xi_j^z(t)}{2}\right) \right\rangle_\phi$$

Large deviation form

$$A(t) = \left\langle \exp\left(-\frac{N\chi^z(t)}{2}\right) \right\rangle_\phi \qquad \chi^\alpha(t) \equiv N^{-1} \sum_j \xi_j^\alpha(t)$$

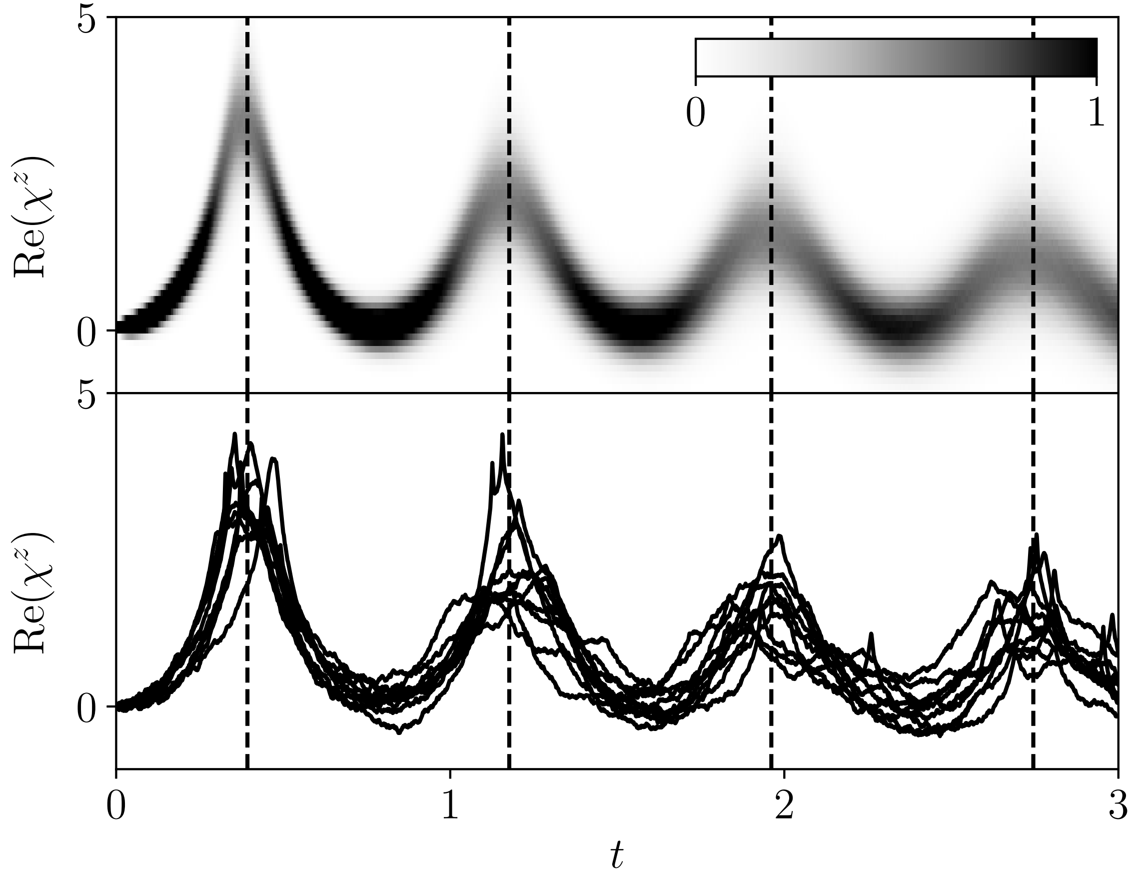
$$A(t) = \left\langle e^{-\frac{N\mathrm{Re}\chi^z(t)}{2}} e^{-\frac{iN\mathrm{Im}\chi^z(t)}{2}} \right\rangle_\phi$$

$$\lambda(t) = -N^{-1} \ln |A(t)|^2$$

Loschmidt peaks in $\lambda(t)$ are turning points of $|A(t)|$

Turning points of $|A(t)|$ expected near turning points of $\mathrm{Re}\langle\chi^z(t)\rangle_\phi$

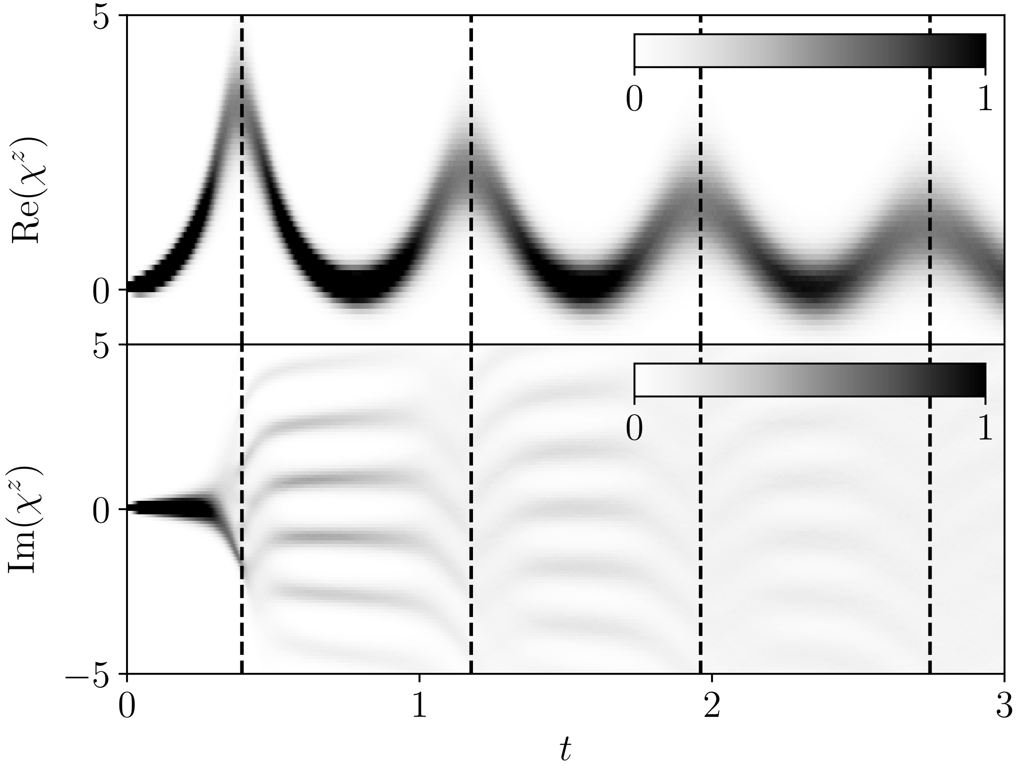
Distribution of $\mathrm{Re}\,\chi^z(t)$



Turning points of $\mathrm{Re}\langle\chi^z(t)\rangle_\phi$ close to Loschmidt peaks

Distribution of Classical Variables

Distributions of $\mathrm{Re}(\chi^z)$ and $\mathrm{Im}(\chi^z)$ show signatures of DQPTs



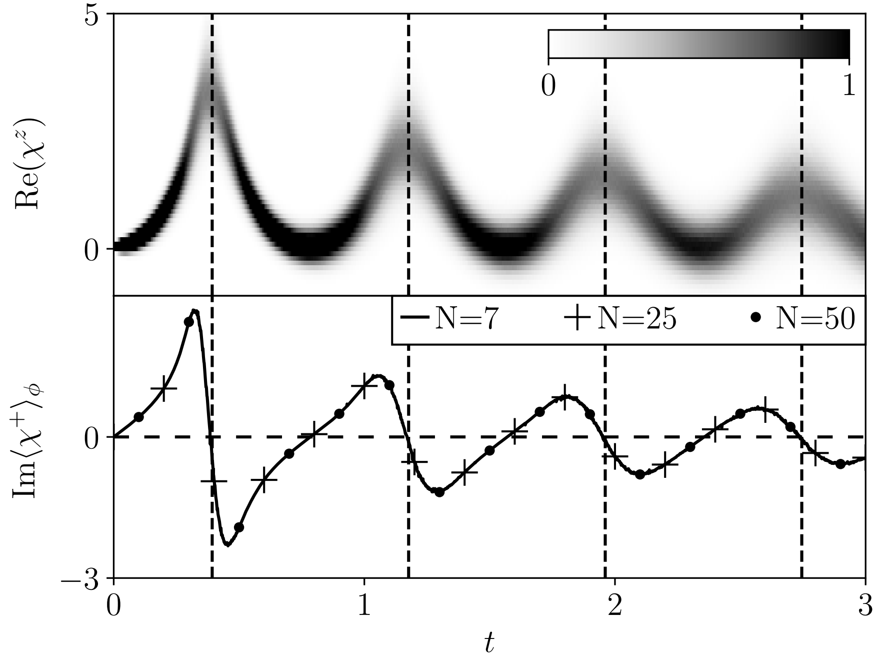
Turning points of $\mathrm{Re}\langle\chi^z(t)\rangle_\phi$ close to Loschmidt peaks

Turning Points of $\mathrm{Re}\langle\chi^z(t)\rangle_\phi$

Ising SDEs yield

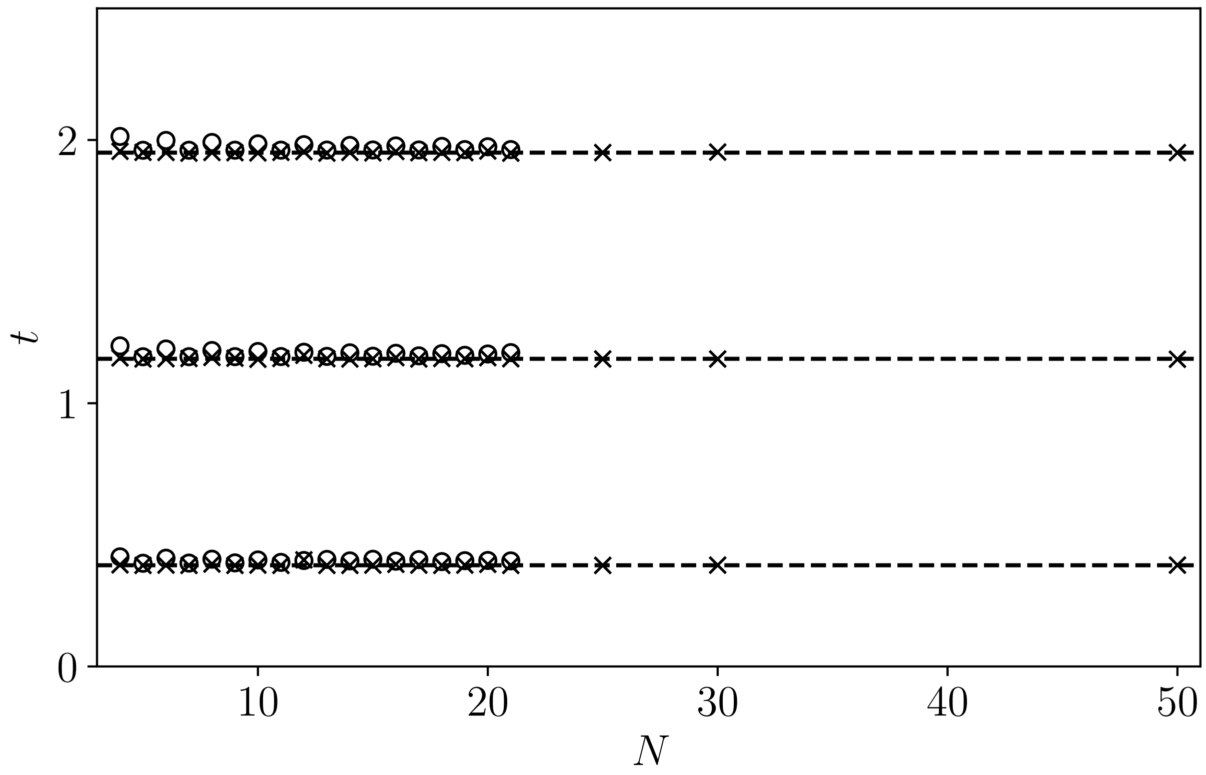
$$\langle\dot{\chi}^z(t)\rangle_\phi = -i\Gamma\langle\chi^+(t)\rangle_\phi$$

Turning points of $\langle\chi^z(t)\rangle_\phi$ correspond to zeros of $\mathrm{Im}\langle\chi^+(t)\rangle_\phi$



Zeros of $\mathrm{Im}\langle\chi^+(t)\rangle_\phi$ close to Loschmidt peaks

Zeros of $\langle \chi^+(t) \rangle_\phi$

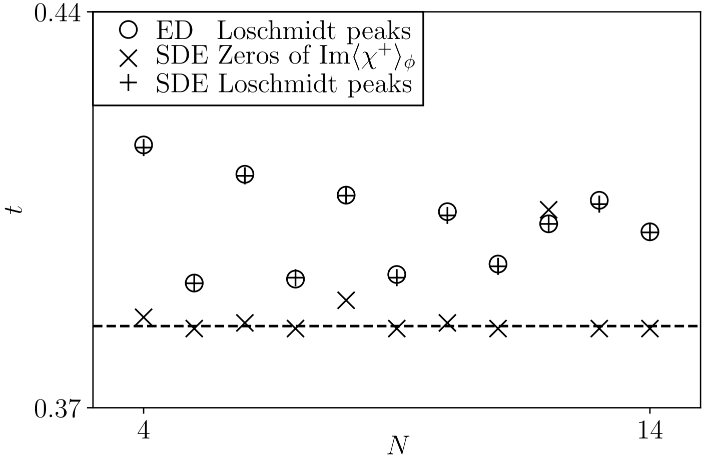


Almost no dependence on system size

$\times$ SDE Zeros of $\mathrm{Im}\langle \chi^+(t) \rangle_\phi$ $\circ$ ED Loschmidt peaks

Comparison to Exact Diagonalization

Turning of $\mathrm{Re}\langle\chi^z(t)\rangle_\phi$ close to, but not exactly at Loschmidt peaks



Need to include imaginary parts of $\chi^z(t)$

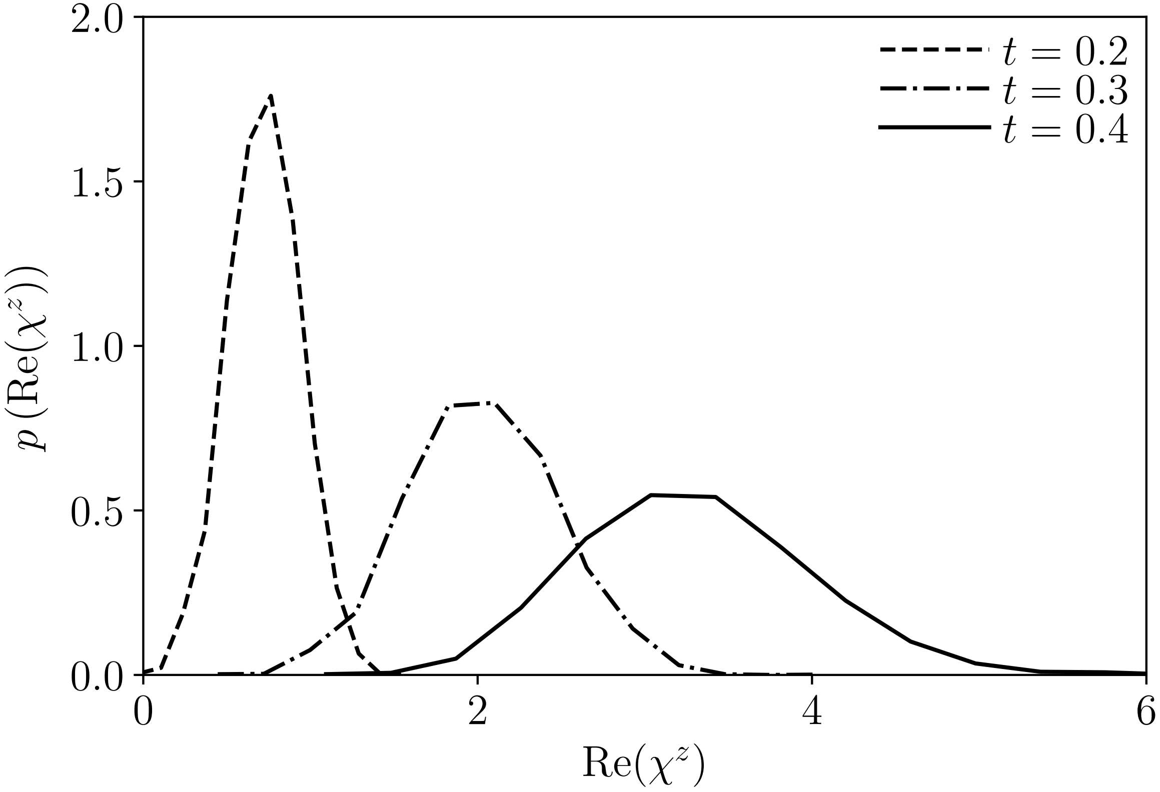
$$A(t) = \left\langle \exp\left(-\frac{N\chi^z(t)}{2}\right) \right\rangle_\phi$$

Complete average including $\mathrm{Re}\,\chi^z(t)$ **and** $\mathrm{Im}\,\chi^z(t)$ **using the SDEs gives an exact match to ED**

Dependence of $\mathrm{Im}\,\chi^z(t)$ on N might illuminate finite-size effects

Enhanced Fluctuations Near Transitions

$N = 7$ spins



Classical distribution broadens on approaching DQPTs

2D Quantum Ising Model

$$\hat{H}_{\rm I}^{\rm 2D} = -J \sum_{\langle \mathbf{ij} \rangle} \hat{S}_{\mathbf{i}}^z \hat{S}_{\mathbf{j}}^z - \Gamma \sum_{\mathbf{i}} \hat{S}_{\mathbf{i}}^x$$

$$\Gamma_c^{\rm 2D} \sim 1.523 J$$

Pfeuty & Elliot (1971)   du Croo de Jongh & van Leeuwen (1998)

Initialise system in ferromagnetic state $|\Downarrow\rangle$

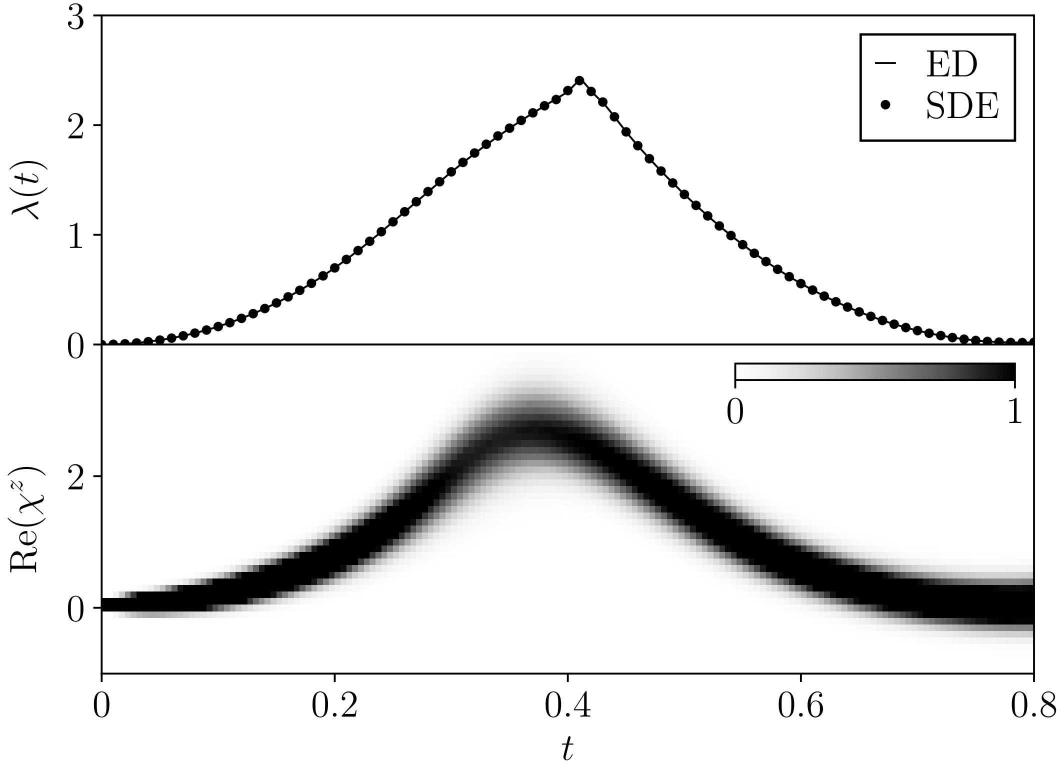
Loschmidt amplitude given by 2D extension of 1D result

$$A(t) = \left\langle \prod_{\mathbf{i}} \exp\left(-\frac{\xi_{\mathbf{i}}^z(t)}{2}\right) \right\rangle_\phi$$

2D Loschmidt Amplitude

3×5 spin system

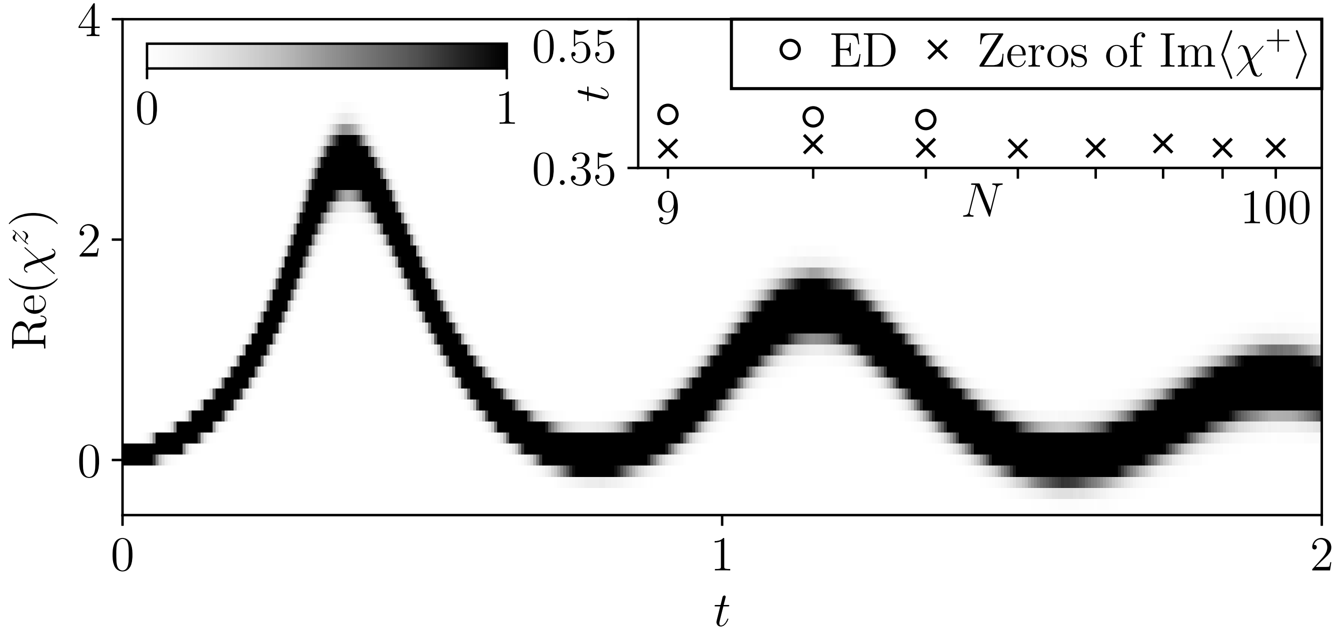
Quench from $\Gamma = 0$ to $\Gamma = 8J$ across 2D QCP at $\Gamma_c^{2D} \sim 1.523J$



Excellent agreement with ED with peak in classical distribution

Classical Distribution for Large System

10×10 spin system



Signatures of DQPTs seen in classical distribution

Features of Stochastic Approach

- Approach based on equations allows access to formulae
- Applies to integrable and non-integrable problems
- Higher dimensions
- Readily parallelized
- Link between quantum and classical processes
- Opens door to other techniques
- Large deviations, enhanced sampling ...
- Classical insights into quantum problems

Conclusions

Non-Equilibrium Dynamics of Quantum Spin Systems

Developed SDE approach into a viable tool for studying integrable and non-integrable spin problems

Signatures of DQPTs in classical distributions

Higher Dimensions

Loschmidt amplitude in 2D

Work in Progress

Large deviations, ground states, XXZ, higher S, open systems ...

Acknowledgements

Sam Begg, George Booth, John Chalker, Andrew Green, Vladimir Gritsev and Lev Kantorovich

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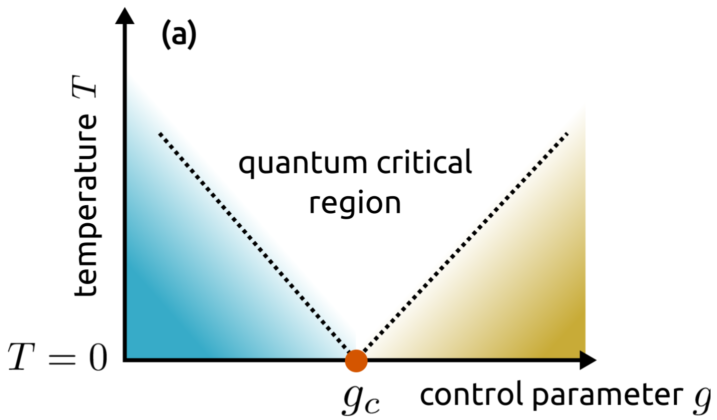
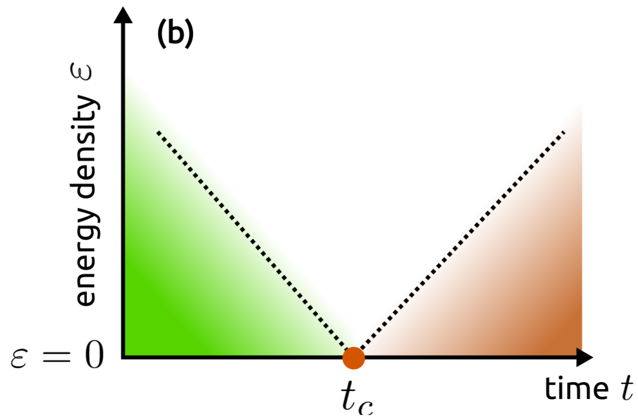
Dynamical Quantum Phase Transitions



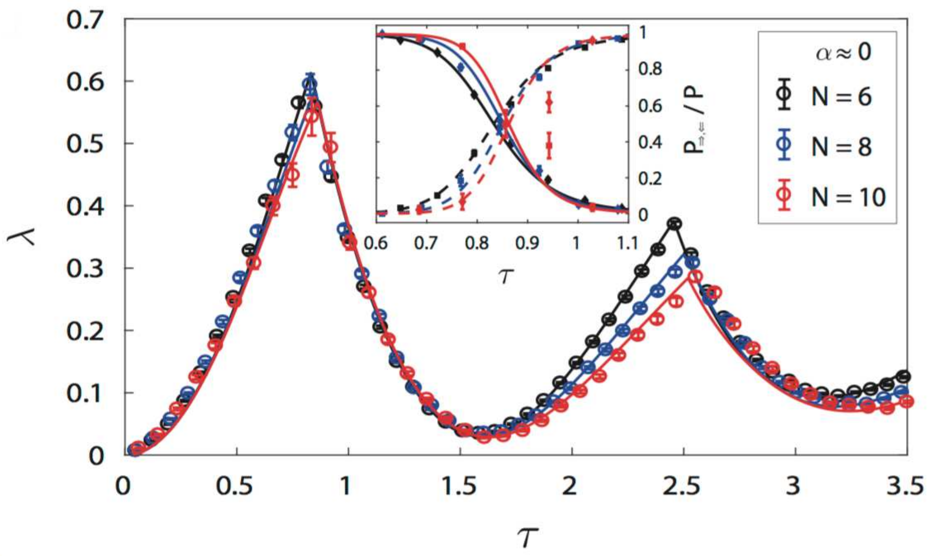


Markus Heyl, *"Dynamical quantum phase transitions: a review"*,

Rep. Prog. Phys. **81**, 054001 (2018)

Innsbruck Experiments

Jurcevic, Shen, Hauke, Maier, Brydges, Hempel, Lanyon, Heyl, Blatt and Roos, *Direct observation of dynamical quantum phase transitions in an interacting many-body system*, Phys. Rev. Lett. **119**, 080501 (2017)



Trapped-ion quantum simulator

$$\hat{H} = -\hbar \sum_{i<j}^{N} J_{ij} \hat{\sigma}_i^x \hat{\sigma}_j^x - \hbar B \sum_i^N \hat{\sigma}_i^z$$

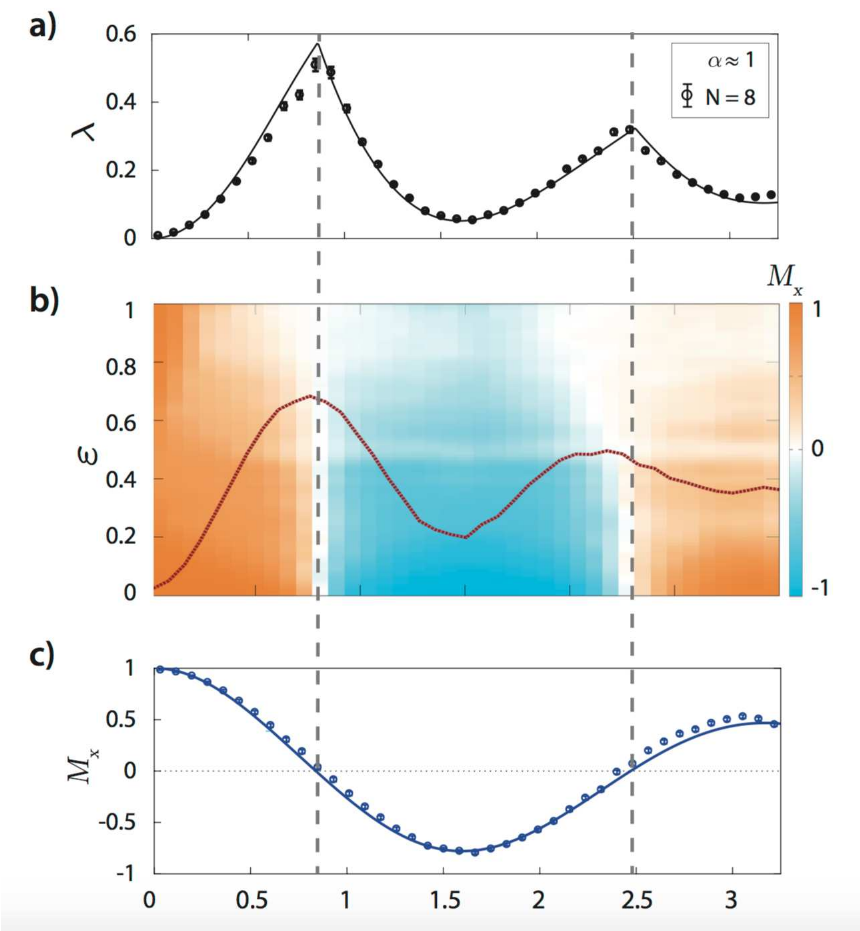
$$J_{ij} \sim \frac{J_{i,i+1}}{|i-j|^\alpha}$$

$$0 < \alpha < 3$$

Quantum quench from FM to PM

Magnetization Dynamics

Jurcevic *et al*, Phys. Rev. Lett. **119**, 080501 (2017)

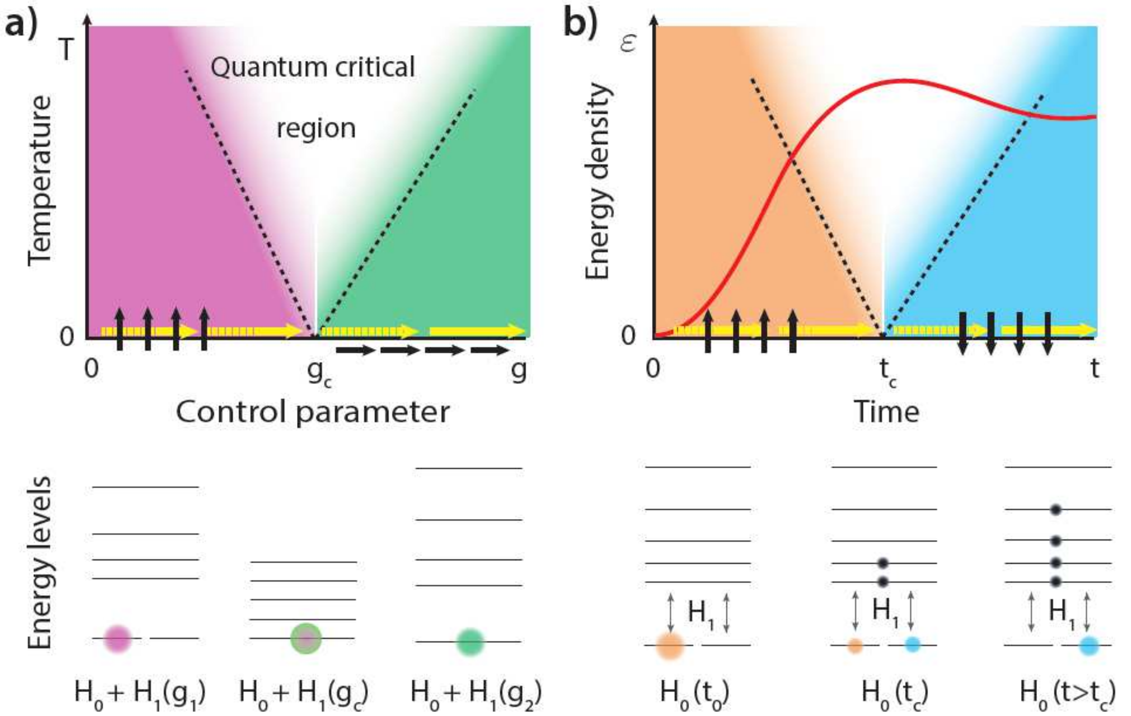


Signatures of DQPTs in other physical observables

Magnetization Dynamics

Jurcevic *et al*, Phys. Rev. Lett. **119**, 080501 (2017)

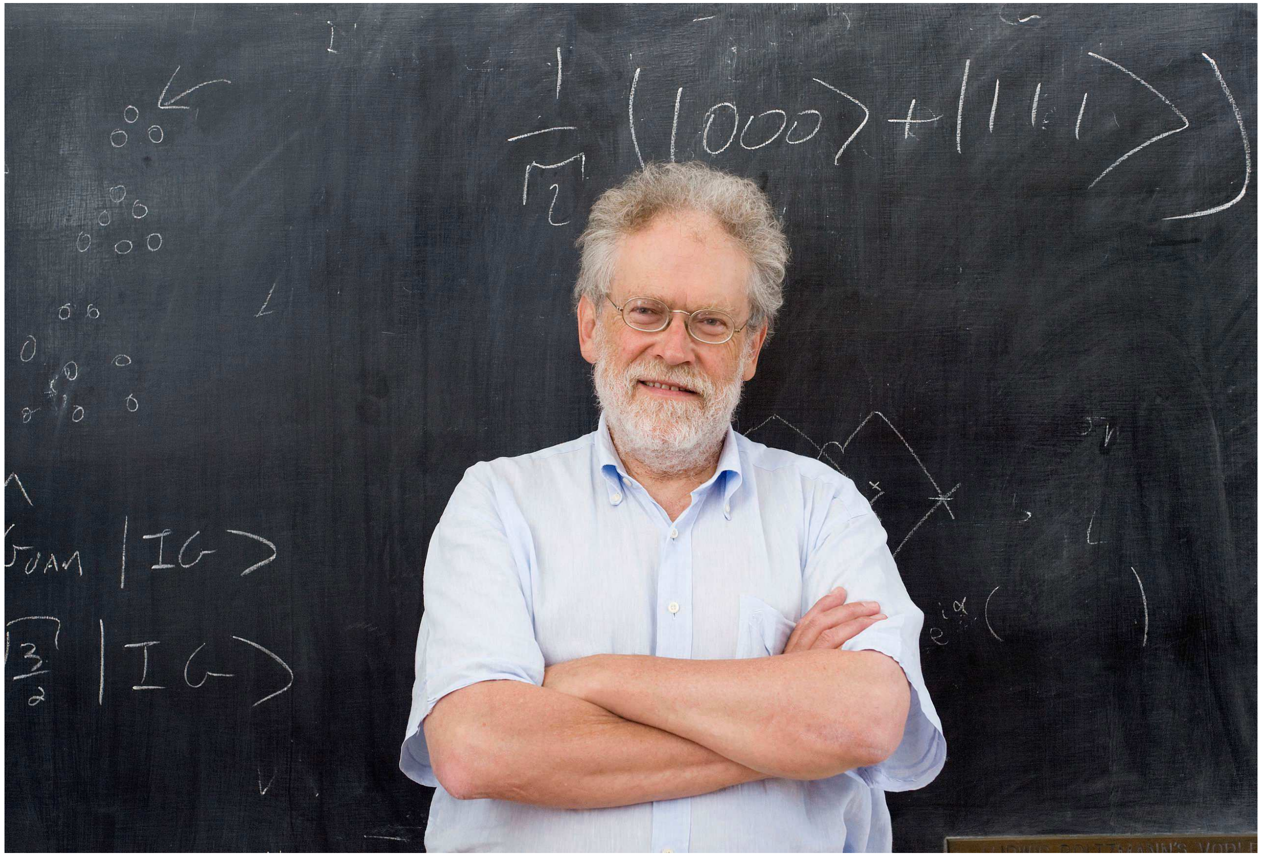
Heyl, Phys. Rev. Lett. **113**, 205701 (2014)



At t_c system is in a Greenberger-Horne-Zeilinger (GHZ) state

$$\frac{1}{\sqrt{2}}\left(|\Uparrow\rangle + |\Downarrow\rangle\right) \qquad |\Uparrow\rangle = |\uparrow\uparrow\uparrow\ldots\rangle \qquad |\Downarrow\rangle = |\downarrow\downarrow\downarrow\ldots\rangle$$

Anton Zeilinger



https://en.wikipedia.org/wiki/Anton_Zeilinger

Other Observables

Local magnetization

$$\langle \hat{S}_i^z(t) \rangle = \langle \psi(0)|\hat{U}^\dagger(t)\hat{S}_i^z\hat{U}(t)|\psi(0)\rangle$$

Forwards and backwards time-evolution operators

Decoupled by two Hubbard–Stratonovich variables, ϕ_i^a and $\tilde{\phi}_i^a$, with corresponding disentangling variables $\xi_i^a(\phi)$ and $\tilde{\xi}_i^a(\tilde{\phi})$

$$\langle \hat{S}_i^z(t) \rangle = \left\langle f_i\left(\xi(t), \tilde{\xi}(t)\right) \right\rangle_{\phi,\tilde{\phi}}$$

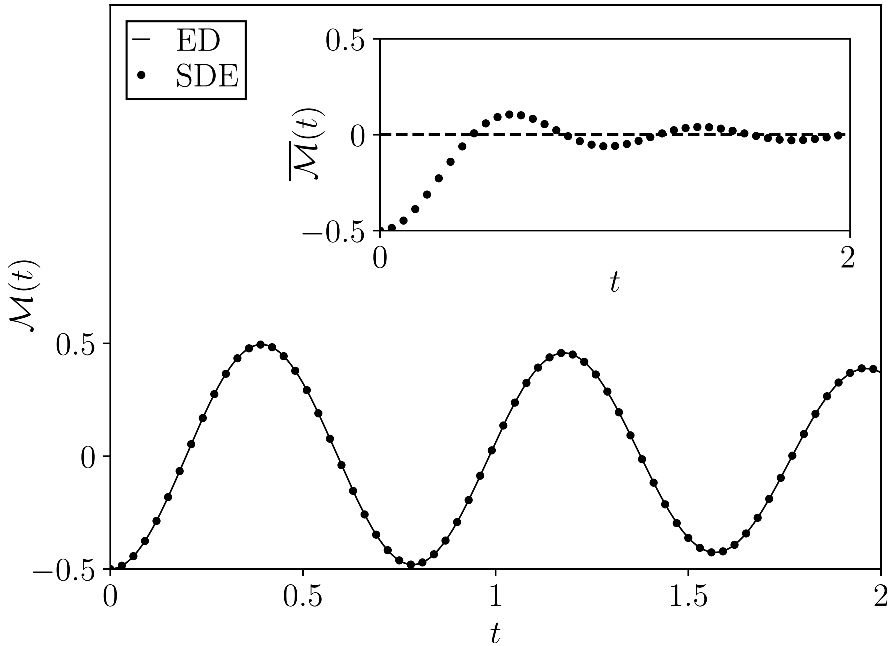
$$f_i = -\frac{1}{2} e^{-\sum_j \frac{\xi_j^z + (\tilde{\xi}_j^z)^*}{2}} [1 - \xi_i^+ (\tilde{\xi}_i^+)^*] \prod_{j \neq i} [1 + \xi_j^+ (\tilde{\xi}_j^+)^*]$$

Magnetization Dynamics

Integrable Ising model with $h = 0$

$$\mathcal{M}(t) \equiv N^{-1} \sum_{i=1}^{N} \langle \hat{S}_i^z(t) \rangle \qquad \overline{\mathcal{M}}(t) \equiv t^{-1} \int_0^t \mathrm{d}s \, \mathcal{M}(s)$$

Quantum quench from $\Gamma = 0$ to $\Gamma = 16\Gamma_c$ with $N = 3$



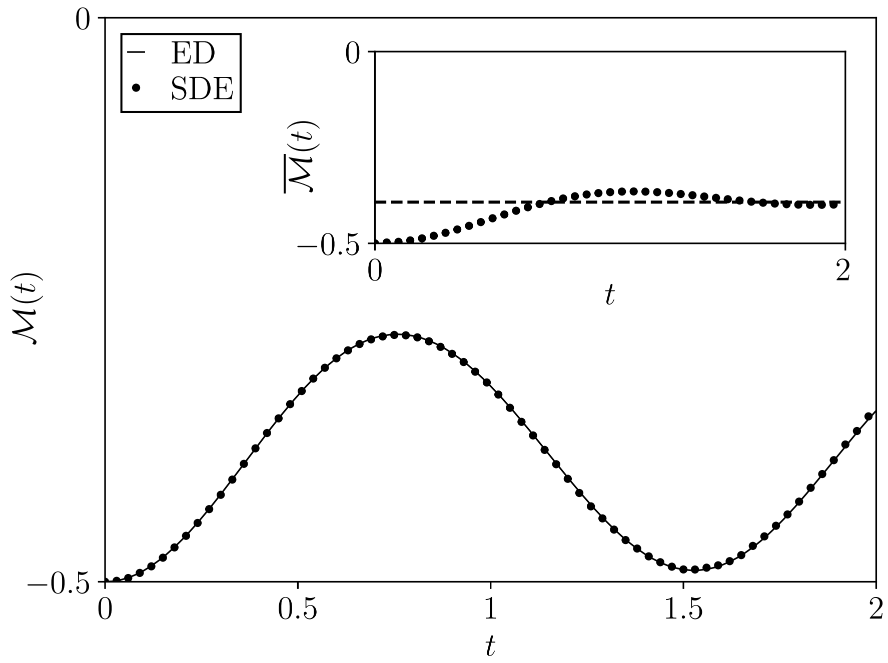
$\overline{\mathcal{M}}(t) \to 0$, as expected for $h = 0$

Magnetization Dynamics

Non-integrable Ising model with $h \neq 0$

$$\mathcal{M}(t) \equiv N^{-1} \sum_{i=1}^{N} \langle \hat{S}_i^z(t) \rangle \qquad \overline{\mathcal{M}}(t) \equiv t^{-1} \int_0^t \mathrm{d}s\, \mathcal{M}(s)$$

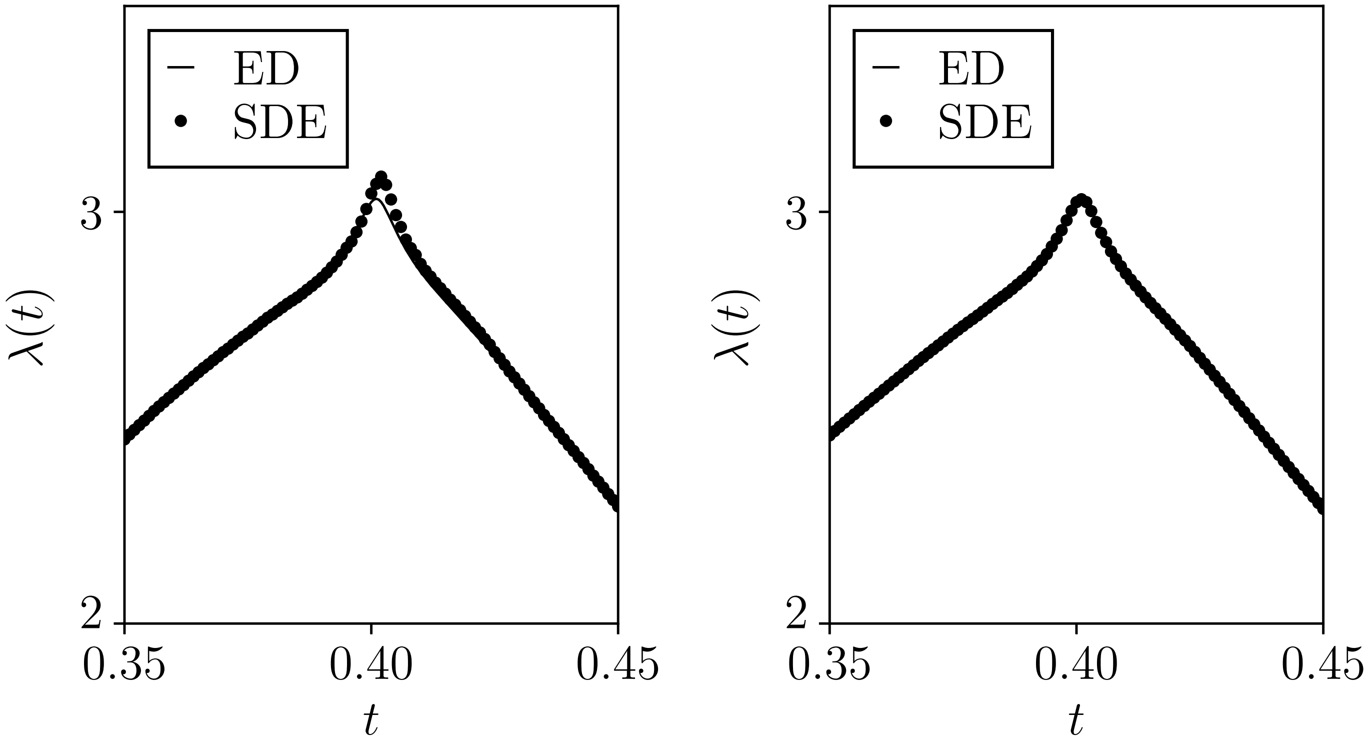
Quantum quench from $\Gamma = 0$ to $\Gamma = 2J$ with $h = 3J$ and $N = 3$



$\overline{\mathcal{M}}(t) \to$ constant, as expected for $h \neq 0$

Number of Stochastic Realizations

$N = 14$ spins



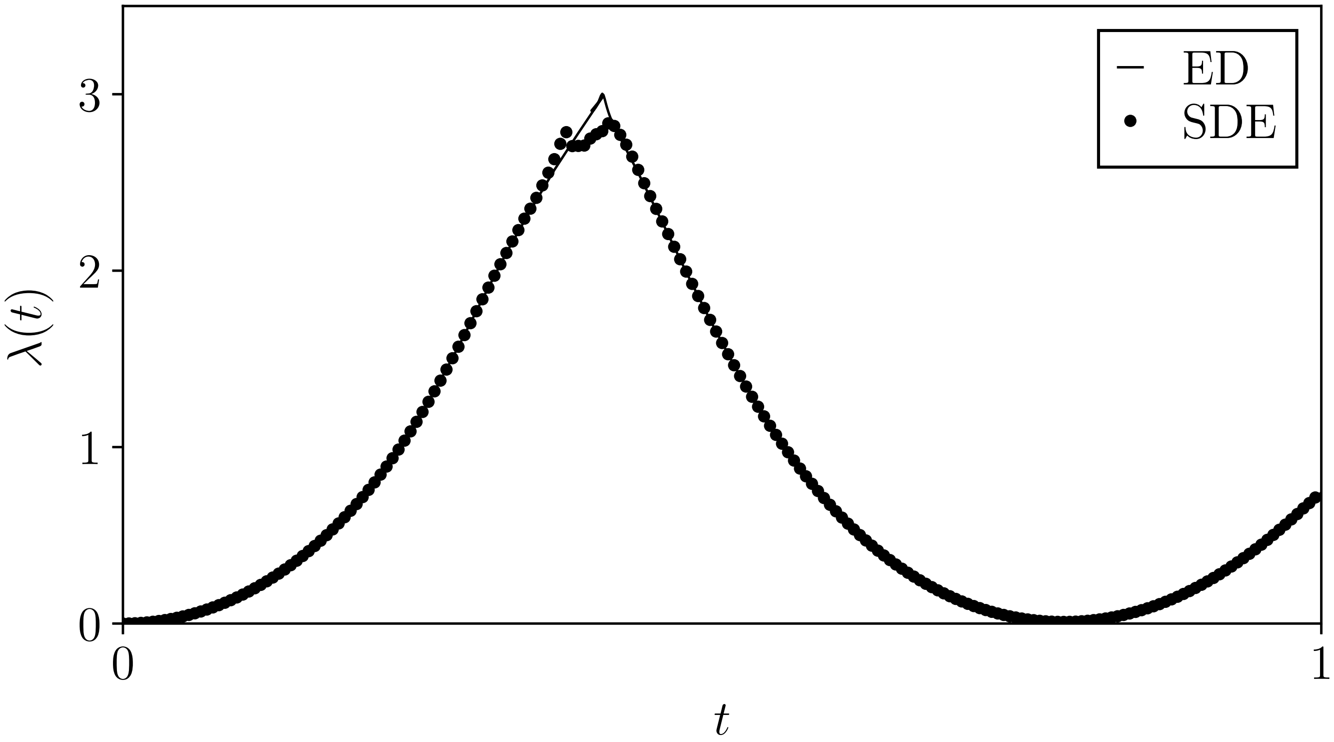
3×10^5 versus 3×10^6 stochastic realizations

SDE comes back to ED result, even when peak is not resolved

Exact method - just to need to sample properly

Larger Spin Systems

$N = 21$ spins

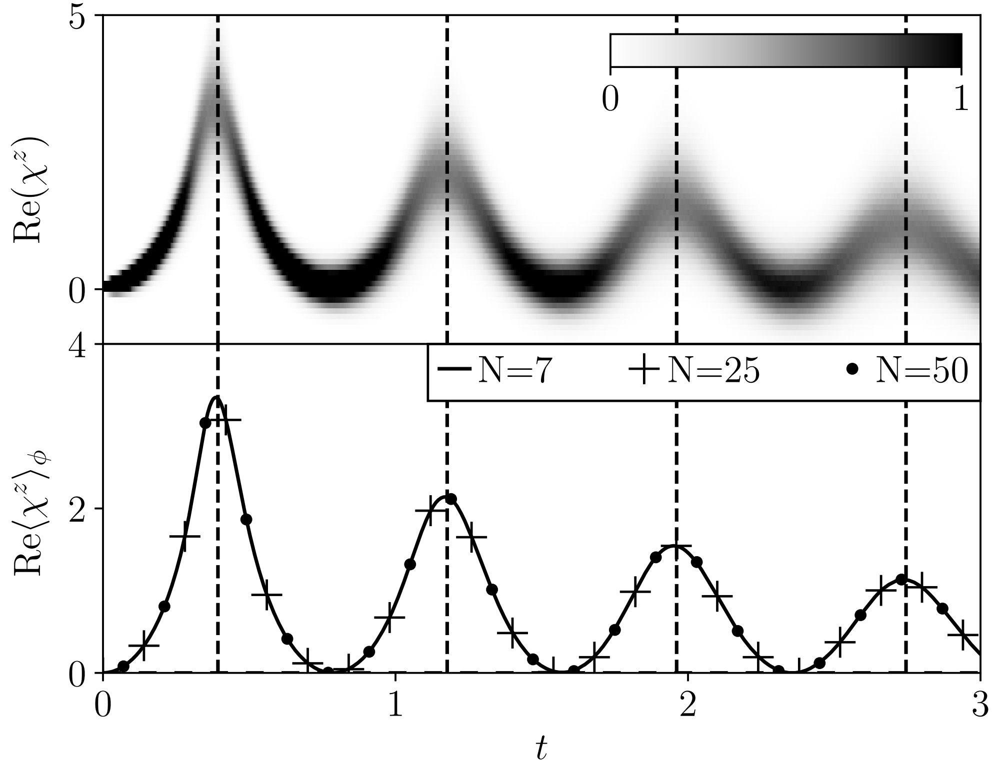


5×10^6 stochastic realizations

SDE comes back to ED result, even when peak is not resolved

Exact method - just to need to sample properly

Different System Sizes



Average of classical distribution has little dependence on N

Applies to entire evolution not just turning points

Main Message

Exact reformulation of quantum dynamics in terms of classical stochastic differential equations

Decouple interactions using Hubbard-Stratonovich

Disentangle evolution operator using group theory

[Note that it depends on the algebra, not the representation]

Next stage

Obtain expressions for physical observables in terms of ξ_j^a

Solve the SDEs

Classical averages yield quantum expectation values